L-Università ta' Malta

Department of Chemistry
Faculty of Science

B.Sc. (Hons.) Year I

Sample Coursework Assignment

CHE1215: Methods of Chemical Calculations March 2022

Instructions

This assignment will assess your knowledge of the topics we have covered so far in class, namely basic algebra, trigonometry, functions, differentiation and integration.

Read the following instructions carefully.

- This assignment carries a small percentage of your final mark for the course.
- This assignment consists of **6 questions** and is out of **100 marks**.
- Submit your solutions in PDF format (handwritten & scanned) on VLE by **Thursday, 31st of March, 2022**, no later than 23:55.
- Attempt **all** questions.

⚠ This is not a group assignment: plagiarism will not be tolerated.

MATHEMATICAL FORMULÆ

ALGEBRA

Factors

$$a^3 + b^3 = (a+b)(a^2 - ab + b^2)$$
$$a^3 - b^3 = (a-b)(a^2 + ab + b^2)$$

Quadratics

If $ax^2 + bx + c$ has roots α and β,

$$\Delta = b^2 - 4ac$$
$$\alpha + \beta = -\tfrac{b}{a} \qquad \alpha\beta = \tfrac{c}{a}$$

Finite Series

$$\sum_{k=1}^{n} 1 = n \qquad \sum_{k=1}^{n} k = \frac{n(n+1)}{2}$$
$$\sum_{k=1}^{n} k^2 = \frac{k(k+1)(2k+1)}{6}$$
$$(1+x)^n = \sum_{k=0}^{n} \binom{n}{k} x^n$$
$$= 1 + nx + \tfrac{n(n-1)}{2\cdot 1} x^2 + \cdots + x^n$$

GEOMETRY & TRIGONOMETRY

Distance Formula

If $A = (x_1, y_1)$ and $B = (x_2, y_2)$,

$$d(A,B) = \sqrt{(x_1 - x_2)^2 + (y_1 - y_2)^2}$$
$$= \sqrt{\Delta x^2 + \Delta y^2}$$

Pythagorean Identity

$$\cos^2\theta + \sin^2\theta = 1$$

General Solutions

$$\cos\theta = \cos\alpha \iff \theta = \pm\alpha + 2\pi\mathbb{Z}$$
$$\sin\theta = \sin\alpha \iff \theta = (-1)^n\alpha + \pi n, \ n \in \mathbb{Z}$$
$$\tan\theta = \tan\alpha \iff \theta = \alpha + \pi\mathbb{Z}$$

CALCULUS

Derivatives

$f(x)$	$f'(x)$
x^n	nx^{n-1}
$\sin x$	$\cos x$
$\cos x$	$-\sin x$
$\tan x$	$\sec^2 x$
$\cot x$	$-\operatorname{cosec}^2 x$
$\sec x$	$\sec x \tan x$
$\operatorname{cosec} x$	$-\operatorname{cosec} x \cot x$
e^x	e^x
$\log x$	$1/x$
uv	$u'v + uv'$
u/v	$(u'v - uv')/v^2$

Integrals

$f(x)$	$\int f(x)\,dx$
$x^n\ (n \neq -1)$	$\frac{x^{n+1}}{n+1}$
$\sin x$	$-\cos x$
$\cos x$	$\sin x$
$\tan x$	$\log(\sec x)$
$\cot x$	$\log(\sin x)$
$\sec x$	$\log(\sec x + \tan x)$
$\operatorname{cosec} x$	$\log(\tan \frac{x}{2})$
e^x	e^x
$1/x$	$\log x$
$\frac{1}{a^2+x^2}$	$\frac{1}{a}\tan^{-1}\left(\frac{x}{a}\right)$
$\frac{x}{\sqrt{a^2+x^2}}$	$\sin^{-1}\left(\frac{x}{a}\right)$

Homogeneous Linear Second Order ODEs

If the roots of $ak^2 + bk + c$ are k_1 and k_2, then the differential equation $ay'' + by' + cy = 0$ has general solution

$$y(x) = \begin{cases} c_1 e^{k_1 x} + c_2 e^{k_2 x} & \text{if } k_1 \neq k_2 \\ c_1 e^{kx} + c_2 x e^{kx} & \text{if } k = k_1 = k_2 \\ e^{\alpha x}(c_1 \cos\beta x + c_2 \sin\beta x) & \text{if } k = \alpha \pm \beta i \in \mathbb{C} \end{cases}$$

Infinite Series

$$e^x = \sum_{n=0}^{\infty} \frac{x^n}{n!} = 1 + x + \frac{x^2}{2} + \frac{x^3}{3!} + \frac{x^4}{4!} \cdots$$
$$\cos x = \sum_{\substack{n=0 \\ n \text{ even}}}^{\infty} \frac{(-1)^{\frac{n}{2}}}{n!} x^n = 1 - \frac{x^2}{2} + \frac{x^4}{4!} - \cdots$$
$$\sin x = \sum_{\substack{n=1 \\ n \text{ odd}}}^{\infty} \frac{(-1)^{\frac{n-1}{2}}}{n!} x^n = x - \frac{x^3}{3!} + \frac{x^5}{5!} - \cdots$$
$$\log(1+x) = \sum_{n=1}^{\infty} \frac{(-1)^{n+1}}{n} x^n = x - \frac{x^2}{2} + \frac{x^2}{3} - \cdots, \quad x \in (-1, 1]$$

1. Consider the function $f(x, y, z) = x^2y + 2xyz + 3xz^2$.

   (a) Determine the partial derivatives $\frac{\partial f}{\partial x}$, $\frac{\partial f}{\partial y}$ and $\frac{\partial f}{\partial z}$.

   (b) Find the total differential, df.

   (c) The *Hessian matrix* **H** of f is the following 2D table of partial derivatives:

$$\mathbf{H} = \begin{pmatrix} \frac{\partial^2 f}{\partial x^2} & \frac{\partial^2 f}{\partial x \partial y} & \frac{\partial^2 f}{\partial x \partial z} \\ \frac{\partial^2 f}{\partial y \partial x} & \frac{\partial^2 f}{\partial y^2} & \frac{\partial^2 f}{\partial y \partial z} \\ \frac{\partial^2 f}{\partial z \partial x} & \frac{\partial^2 f}{\partial z \partial y} & \frac{\partial^2 f}{\partial z^2} \end{pmatrix}.$$

   Compute the partial derivatives that should go in this matrix, and write your final answer in the form of a 3×3 grid as above.

[3, 2, 9 marks]

2. (a) Determine the derivative of each of the following functions.

   (i) $y = 7x^4 + 5x^2 - 1 + \frac{1}{3x} + \frac{5}{4x^3}$

   (ii) $y = 2\sin(3x)$

   (iii) $y = \sin(x^2 + 1)$

   (iv) $y = \sin\sqrt{x^2 + 1}$

   (v) $y = (x^2 + 1)\sin x$

   (vi) $y = \frac{\sin x}{x^2 + 1}$

   (vii) $y = \log \frac{\sqrt{\sin\sqrt{x}}}{\sqrt[3]{e^{5x+1}}}$

   (b) The probability that a molecule of mass m in a gas at temperature T has speed v is given by the Maxwell–Boltzmann distribution

$$f(v) = 4\pi\left(\frac{m}{2\pi kT}\right)^{3/2} v^2 e^{-\frac{mv^2}{2kT}},$$

   where k is Boltzmann's constant. What is the most probable speed (i.e., the speed v for which $f(v)$ is maximised)?

[14, 5 marks]

3. A polynomial function f is given by

$$f(x) = 1 + (2+3x)(4x+5)^2.$$

(a) Find the remainder when f is divided by:

(i) $x-1$,

(ii) x^2-1.

(b) Give a full factorisation of f. Hence determine all solutions to

$$4x+5 = -\frac{1}{(2+3x)(4x+5)}.$$

(c) Determine the coordinates of the stationary points on the curve $y = f(x)$, and state their nature.

(d) Hence, give a sketch of $y = f(x)$, labelling any turning points and intercepts with the coordinate axes.

(e) Using partial fractions, show that

$$\int \frac{10}{f(x)}\,dx = \log\left(\frac{\sqrt[4]{(4x+3)^5(12x+17)^3}}{(x+1)^2}\right) + c,$$

where log denotes the natural logarithm.

[4, 3, 4, 3, 12 marks]

4. Find the general and particular solutions to the following differential equations.

(a) $\dfrac{dy}{dx} = y^2 \sin x$, given that $y = 1$ when $x = 0$.

(b) $\dfrac{dy}{dx} = e^{x-y}$, given that $y = 0$ when $x = 0$.

(c) $\dfrac{d^2y}{dx^2} + 2\dfrac{dy}{dx} - 3y = e^{2x}$, given that $y = 0$ and $\dfrac{dy}{dx} = 1$ when $x = 0$.

[5, 5, 8 marks]

5. Consider the quadratic expression $g(x) = 4x^2 + 4x - 15$.

   (a) Express $g(x)$ in the form $a(x-p)^2 + q$ for appropriate values of a, p and q.

   (b) Hence, sketch the graph of $y = g(x)$, clearly labelling any turning points and intercepts with the coordinate axes.

[4, 4 marks]

6. (a) Let $A = (1,2)$ and $B = (-3,7)$ be two points in 2D.

      (i) Find the distance between A and B.

      (ii) Find the equation of the straight line passing through the points A and B.

   (b) Solve the equation $\cos\vartheta = \frac{1}{2}$ for angles $-2\pi \leqslant \vartheta \leqslant 2\pi$. Sketch your solutions on the unit circle.

   (c) Solve the equations

$$\begin{cases} 3^{x+y} = 9^{9x+5} \\ \log_{3x+2}(3x^2 + y) = 2 \end{cases}$$

   simultaneously.

[5, 5, 5 marks]